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COMPUTER SCIENCE CENTER

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Computer-Oriented Research in the Space Related Sciences at the University of Maryland

by

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In March 1963, the National Aeronautics and Space Administration awarded Research Grant NsG-398 to the Computer Science Center of the University of Maryland. This grant is entitled "Computer-Oriented Research in the Space Related Sciences" and is in support of a multidisciplinary research program concerned with the application of modern high-speed digital computers to research projects in a broad spectrum of the space related sciences. In particular, this program is aimed at stimulating and broadening the effective use of computers in the University's space related efforts and at investigating new methods of computer application in these fields.

When a computer is used as part of a research project, the high cost of the necessary equipment, problems of receiving proper programming help, etc., often overshadow the entire computational effort and overstress the service nature of the computer work. However, more and more research investigators have become aware of the fact that this service aspect should not be the major consideration in the application of computers to their work. Rather, a highly significant and important contribution stems from the fact that the analysis undertaken to make possible the assistance of computers will often stimulate a type of feedback that casts new light on the research problem itself; thereby, in turn furthering the research effort. At the same time, challenging research problems often arise concerning methods and concepts of computer-application in general; in other words, concerning relevant problems in computer science. The research program therefore aims to stimulate this type of thorough analysis in the computer science aspects of the University's space research projects, thereby making the investigators aware of new possibilities and potentially new approaches to their problems as provided by the computer. In support of this effort a research program has been started on a number of problems in computer science, in order to deepen our knowledge and understanding of the methods and ideas underlying the use of computers in research.

The main responsibility for the research program is carried by the Computer Science Center of the University of Maryland. The Center is an interdisciplinary research department of the University of Maryland, not associated with any college or school within the University. The Center now also offers a number of regular undergraduate University courses in computer science and plans are under way to establish a graduate degree program in this field. In cooperation with the NASA-Goddard Space Flight Center and The Catholic University of America, the Center also conducts a regular seminar and colloquium series on special topics in computer science.

Figure 1 provides a brief list of principal facts about the Center. Not counting the graduate assistants and the operational staff, etc., there are 33 full-and-part-time professional staff members of which 15 hold a Ph.D., 8 a Master's, and 7 a Bachelor's degree as highest degree. Of these 33 persons, 18 are presently in some way involved with this research program, representing a full-time equivalent of about 10 people.

In line with the two above mentioned aims of the overall program, there are two distinct areas of work, namely, research in computer science and computer-oriented research in a number of space related disciplines. Figure 2 gives a breakdown of the work presently underway in the first area. For the sake of clarity, this area has been subdivided further into two subareas, one dealing with programming and computing systems, and the other involving more general research projects in computer science. Let me begin by discussing the programming systems work.

Any effective utilization of modern, complex, large-scale computers depends crucially on the availability of versatile programming and monitoring systems. This is especially true when these computers are to serve a multidisciplinary research program such as the one under discussion here, where the proper selection, adaptation, and diversification of highly flexible programming systems is basic to any successful work accomplished under the program. Consequently, one of our first actions was the establishment of a special computer systems group explicitly charged with the selection, implementation and modification of existing systems as well as the design and programming of new systems. It should be stressed that this is a continuous and never-ending task in view of the constantly changing requirements of the individual research projects using the system.

Figure 3 presents a schematic diagram of our main programming system. Several other separate systems are available on request. Basically, we believe that the research user of the machines should be able to use, whenever possible, the appropriate computer

language for his problem. We therefore continue to adapt and incorporate new languages under the system. The hatched areas indicate subsystems which were added to the original IBM-IBSYS monitor by our systems group. Some of them are designed to facilitate use of such highly important languages as IPL-V, OMNITAB, MAD, UMAP, and ALGOL; others represent special developments of multi-precision packages such as MPP and PRECISE; finally, MOIST is a special macro-language for flexible input-output and X-RAY-65 is a subsystem which I shall discuss in a moment. The MAMOS submonitor is our own development, which has proven to be highly flexible and is even now being adapted for use on an IBM-7094-7044 direct couple system at the NASA-Goddard Space Flight Center, and at Yale University.

When a particular research project involves a wide variety of computational aspects, it frequently becomes necessary to combine all these aspects under a special programming system, giving the investigator flexible and ready access to all his programs and providing for automatic data transmission between all of them. As seen on the previous Figure 2, there are three such special systems under development at the Center, one concerning crystallographic structure determination, another one dealing with electrolyte computations, and a third involving special-purpose chemical engineering computations. Let me discuss only one of them, namely the crystallographic system called X-RAY-65.

The problem of determining the structure of crystals is at present one of great interest to chemists, biologists, and geologists. This research project is directly concerned with the development of methods and corresponding computer programs for the accurate determination of the atomic parameters in crystals from X-Ray or neutron diffraction data of solid crystalline material. In the beginning of programming for the solution of crystal structures, it was common practice to write isolated programs for each application. As data gathering techniques improved and became more automated, the need arose to improve and automate the total computational task as well. The programs under development here have accomplished this goal and make up the beginning of a much needed crystallographic computing system.

Figure 4 shows the present extent of the system. The major subroutines perform the calculations necessary to interpret X-Ray diffraction patterns and to establish accurate atomic parameters in crystals. Other programs perform systems-link functions and help in the preparation of data for publication.

Figure 5 shows how a data deck is prepared to control the sequence of the different computations desired by the investigator.

Various control cards direct the automatic flow of data from one program to the next. The cards with an asterisk on the side represent major program calls. For example, DATRDN calls for the application of Lorentz- and polarization corrections and for the encoding of space group information; FC is the structure factor program for all space groups and settings; FOURR is a general three-dimensional Fourier analysis program; DIAGLS, a special and frequently used version of a more general full matrix program, ORFLS, for least-squares analysis; and finally, BONDLA calls for the calculation of bond lengths, angles, inter-atomic and molecular distances, their estimated errors, etc. Among the many possibilities of special data output is a pictorial type output shown in Figure 6, which directly shows the crystalline configuration of the substance.

The X-Ray-65 system is used frequently not only by the University's crystallography group but also by a number of other institutions, including the NASA-Huntsville Space Flight Center, the National Bureau of Standards, and many other research organizations and universities.

Let me now turn to the second area of computer science research. As Figure 2 indicated, several projects are now under active consideration; they concern such widely diverse areas as numerical analysis, automatic image processing, mechanical languages and information storage and retrieval. In view of the time factor, I shall confine myself here to saying only a few words about the first two projects.

In numerical analysis we are primarily interested in the numerical solution of non-linear functional equations. As Figure 7 shows, this particularly concerns non-linear integral and differential equations, and thereby of necessity also non-linear systems of finitely many equations in finitely many unknowns. For theoretical investigations, all these different cases can be subsumed under the general problem of finding and analyzing algorithms for the determination of solutions of a general operator equation in Banach spaces. There is no scarcity for applications in which such non-linear problems occur. Figure 8 lists some of the specific applications that prompted us in part to begin this particular research investigation. To some extent we became aware of the trajectory and control problems as a result of discussions with colleagues at the NASA-Goddard Space Flight Center.

Among the many different methods that can be applied to the non-linear problems here under consideration, we are concerning ourselves particularly with those listed in Figure 9.

The study of Newton's method for general operator equations in Banach spaces originated with the Russian mathematician L. V. Kantorovich. Its application to such specific problems as mentioned earlier presents a variety of challenging research questions which are attracting growing attention in this country. The generalized secant methods are even less understood than the Newton's method and their application - though computationally desirable - present even more serious problems. The Gauss-Seidel and Jacobi-type iterations for non-linear systems of equations appear to carry a great deal of promise for effective computational work, and have only recently come to be considered for use on specific applications. The same is true for the so-called implicit iterations which contain all previously mentioned methods as special cases. All iterative methods require the availability of a suitable initial approximation which in turn must often be already close to the desired solution. Global methods are therefore highly necessary to overcome this restricive condition. Our three areas of work on global methods are also given in Figure 9.

Figure 10 provides a general picture of the particular problems now under active study. It should be stressed that we are working on parallel tracks with the theoretical investigation of all methods and their computational evaluation for specific applications. In addition, we hope to develop versatile programs in a general algorithmic language for all these methods. A number of very promising results have already been obtained, even though this particular project has only been under way for about 6 months.

The earlier mentioned project on Image Processing and Automatic Pattern Recognition concerns several areas of research, listed in Figure 11. Research in digital image processing has tended to be concentrated in two areas: "local" processing of images as two-dimensional data arrays, usually for the purpose of simplifying the image, and processing of images which consist of discrete, well-defined parts in given topological and metric relationships. In the area of the discrimination of connected regions of an image, a general computer program called RAMP has been developed and written, which constitutes an important step toward bridging the gap between the mentioned two "types" of image processing research. RAMP identifies and computes the areas of connected regions - defined by those image points which have a given range of density values - on a digitized image. Figure 12 gives a line-drawing done by hand from a cloud-cover picture, and Figure 13 shows the output of RAMP from the actual digitized picture; unfortunately, in the reproduction process the second figure was rotated by an angle of 90°. Two other image processing techniques were developed and programmed representing alternative

approaches to the problem of identifying regions on an image that are free of detail and have regular boundaries. These programs are called SORD- (which stands for "Solid Region Delineator")-1 and -2. For reasons of time it is not possible to describe the ideas behind all three approaches here. All three programs have been experimentally applied to the problem of analyzing the cloud-cover pictures and maps obtained from the TIROS satellite.

A variety of approaches to the automatic recognition of shapes have been proposed. Under this project, three novel tools for shape description and analysis are being investigated and developed further; namely, the so-called methods of (1) shape skeletons, (2) shape capacity, and (3) shape frames. In each case, versatile computer programs were written and are now being applied to a variety of special problems. The shape skeleton method is particularly interesting; it consists in the "propagation" of the boundary of the shape over the plane in the manner of a wave disturbance. Figure 14 shows a simple line drawing representing a particular shape. Figure 15 gives the actual computer printout of the "propagation" process. Points through which the wave front has passed become "refractory", i.e., resistant to further wave passage. Under these conditions the wave front which propagates inward will intersect itself and eventually cancel itself out. The locus of self-intersections of the propagating waves provides a highly useful "skeletal" representation of the given shape and can be used in succeeding programs to provide detailed information about the shape.

A totally different area of research under this project concerns the problem of visual discrimination of texture by human observers. The appearance of "uniform texture", characteristic of probabilistically-generated visual stimuli suggests that the brain may measure or estimate statistical parameters of such stimuli, as, for example, luminance values and luminance gradients, periodicities of these values, etc. In searching for statistical, stimulus-analysis and -processing mechanisms which may be involved in visual texture perception, it is desirable to study situations involving as few relevant stimulus dimensions as possible. For example, consideration can be restricted to stimuli which are either "black" or "white" at every point. Another, more drastic, restriction to stimuli which are "one-dimensional" can be used to minimize the significance of form and pattern variables, alternatively. A versatile computer program for generating patterns constrained in one direction and random in the other has been developed. Figure 16 presents an output pattern from this program. These patterns are printed out by overstriking up to six printer characters to form the solid black cells. Subjects are shown these patterns and asked to locate boundaries.

Experiments of this type have studied boundary location performance with respect to the very basic mean luminance variable. In other experiments now in progress, mean luminance has been equalized and the variables under study are the frequency distribution of black and white "run lengths" or "patch sizes".

As discussed earlier, the entire research program consists of two parts - computer science research, and research into the computational aspects of particular space-related problems. Figure 17 shows the extent of the second part of the program now in progress. Time permits only a very cursory glance at this fairly extensive, interdisciplinary, research undertaking, since every one of these projects would require considerable time for a description of the physical background and the computational problems involved.

It may be mentioned just in passing that the work listed under Molecular Physics concerns primarily kinetic theory and spectroscopic studies on the fundamental properties of molecules. The heading "Physics and Engineering of Fluids" includes computational work in plasma physics; in particular as it applies to phenomena in the ionosphere and in space, etc., and it also includes problems of magnetohydrodynamics and the flow of gases at high temperatures. The work in astronomy is mainly concerned with radio astronomical observations and galactic and stellar models, while problems in psychology cover such studies as psychomotoric testing of pilots.

Rather than simply enumerating the entire list of topics now under active investigation, let me single out two particular projects. Their choice was dictated largely by the ease with which it is possible to discuss the physical background, rather than for any other reason.

The first of these two projects concerns an <u>in situ</u> probe system for the measurement of ionospheric parameters. For many years now, the ionosphere has been the subject of experimental investigation. The advent of rocket sounding vehicles and satellites has considerably intensified this activity, and at the same time has shifted the experimental emphasis to <u>in situ</u> probes which are, of course, potentially capable of more refined measurements of various ionospheric parameters. For several years, the Center for Atmospheric and Space Physics of the University of Maryland has been conducting a research program aimed at developing a complete <u>in situ</u> probe system in particular. This system consists of, (1) thermal equalization probes capable of independently measuring vehicle potential, (2) a pulse probe to measure electron concentration and energy distribution and (3) a Langmuir probe to supply information on positive ion and

electron temperatures. This system has been completely designed and tested both in the laboratory as well as in preliminary rocket flight tests. A very substantial part of this design and testing work concerned the development of adequate computational approaches to the calculation of instrument behavior and characteristics. Figure 18 shows a picture of one of the thermal equalization probes. It represents essentially a unipotential cathode which, when heated, begins to emit electrons thermionically. In general, the unheated probe in ionospheric plasma assumes a negative potential. When the probe is heated, the outgoing electron flux partially balances the incoming flux of electrons from the plasma, causing a decrease in the probe potential. Figure 19 shows computed curves of potential versus temperature for such a probe. All these curves display a very sharp readily identifiable knee at the plasma potential. A probe whose temperature is set to operate a little above the knee will therefore provide a continuous measure of the vehicle plasma potential. Figure 20 gives actual measurements in flight and shows that the computational results agree very satisfactorily with actual measurements.

Time permitting, I would like to mention as a last project a very extensive experimental and theoretical research study concerning rotating laboratory models which simulate the general circulation of the atmosphere. Figure 21 gives a schematic diagram of the experimental vehicle, a large rotating tank. Fluid is pumped out of the center area and flows back into the tank on its outside rim and, more specifically, into the boundary layer on the bottom of the tank. Dye crystals are dropped from above into the tank in the rim area to trace the circulation. Figures 22 and 23 give a typical picture of this type, taken from above the tank. A very important part of this research program concerns the numerical prediction of such circulations, involving of course the numerical solution of non-linear partial differential equations under fairly general boundary conditions. These circulations are in many respects similar to the general circulation of the atmosphere, and the uses and limitations of numerical methods for the prediction of weather can therefore be tested in these rotating fluid "models". Initial numerical prediction work concerns simple models which permit the parameterization of the viscous boundary layer at the bottom. Figure 24 gives the output from such computations for the perturbation stream function in a cross-section of the tank, about half a radius away from the center. The printout has been arranged in such a way that it is possible to connect equal values in different columns and obtain a graph of the perturbation. The perturbation of course shows the cross-section of vortex-rolls which appear in the particular region. The experimental and the corresponding numerical model is being complicated in successive stages in order

gradually to approach the situation in the atmosphere. For example, as a next step, vertical thermal gradients are now being introduced. Clearly then, the ability to predict laboratory circulations with a given numerical prediction technique will indicate the feasibility of using the same technique for predictions of similar circulations in the atmosphere.

As was stressed several times, it is not possible to give more than a very cursory picture of the work performed under the NASA-Research Grant NsG-398 at the University of Maryland. More detailed descriptions can be found in the various reports and publications that have already originated from the work. In our opinion, the results show very clearly the extreme importance of bringing together computer scientists and research investigators of various space-related problems, thereby stimulating and broadening the work of both.

We are deeply grateful to the National Aeronautics and Space Administration for the understanding and support it has provided for this research program, and I would personally like to extend my sincerest thanks for this support. It is our deepest hope that our work will prove to be useful to the work of NASA and to many other investigators in the space and computer sciences as well.

Statistics of the Computer Science Center of the University of Maryland

Computing Equipment

One IBM-7094-I with 16 tape drives

Two IBM 1401 satellites sharing 6 tape drives with the 7094

Associated off-line card handling equipment

Computer Use

Current average log-time: 590 hours/month ($3\frac{1}{2}$ shifts)

Current average number of production jobs: 6000/month

Personnel

Professorial Faculty	7	Senior Administrative Personnel	3
Part-time Faculty Consultants	9	Programming Staff	14
Graduate Research Assistants	11	Operating Staff	22
NASA Fellows	3	Secretarial Staff	4

Figure 1

Computer Science Research

1. Programming and Computing Systems

   A. General Programming and Monitoring Systems Development

   B. Crystallographic Structure Determination System, X-Ray-65

   C. Programming System for Electrolyte Computations

   D. Special Purpose Chemical Engineering Computing System

2. Computer and Information Science Research

   A. Non-linear Problems of Numerical Analysis

   B. Image Processing and Pattern Recognition

   C. Consequential Languages and Procedures

   D. Information Storage and Retrieval in Depth for a Narrow Field

Figure 2

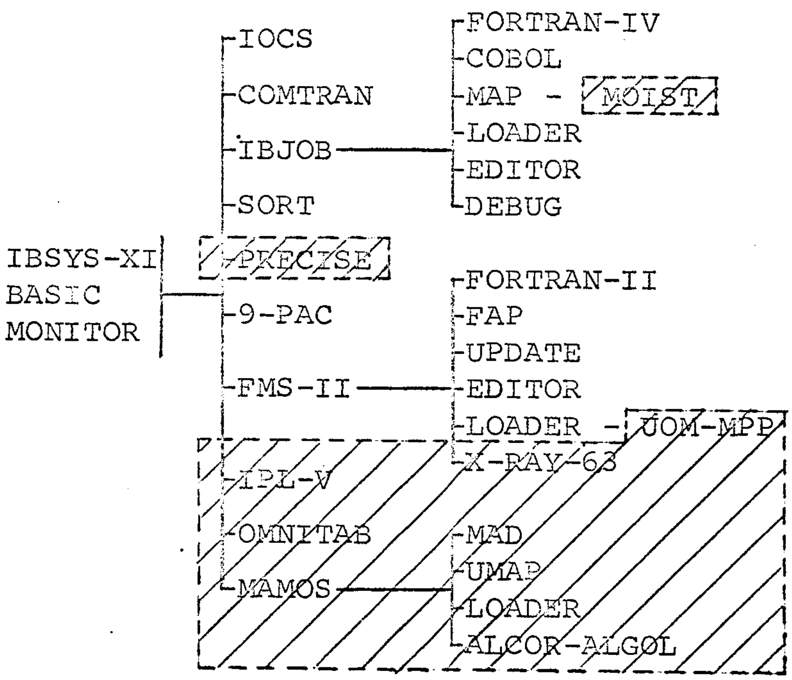

IBSYS-XI
BASIC
MONITOR
IOCS
COMTRAN
IBJOB
SORT
PRECISE
9-PAC
FMS-II
IPL-V
OMNITAB
MAMOS
FORTRAN-IV
COBOL
MAP
MOIST
LOADER
EDITOR
DEBUG
FORTRAN-II
FAP
UPDATE
EDITOR
LOADER
UOM-MPP
X-RAY-63
MAD
UMAP
LOADER
ALCOR-ALGOL

Figure 3

Major Divisions of the X-Ray-65 Systems

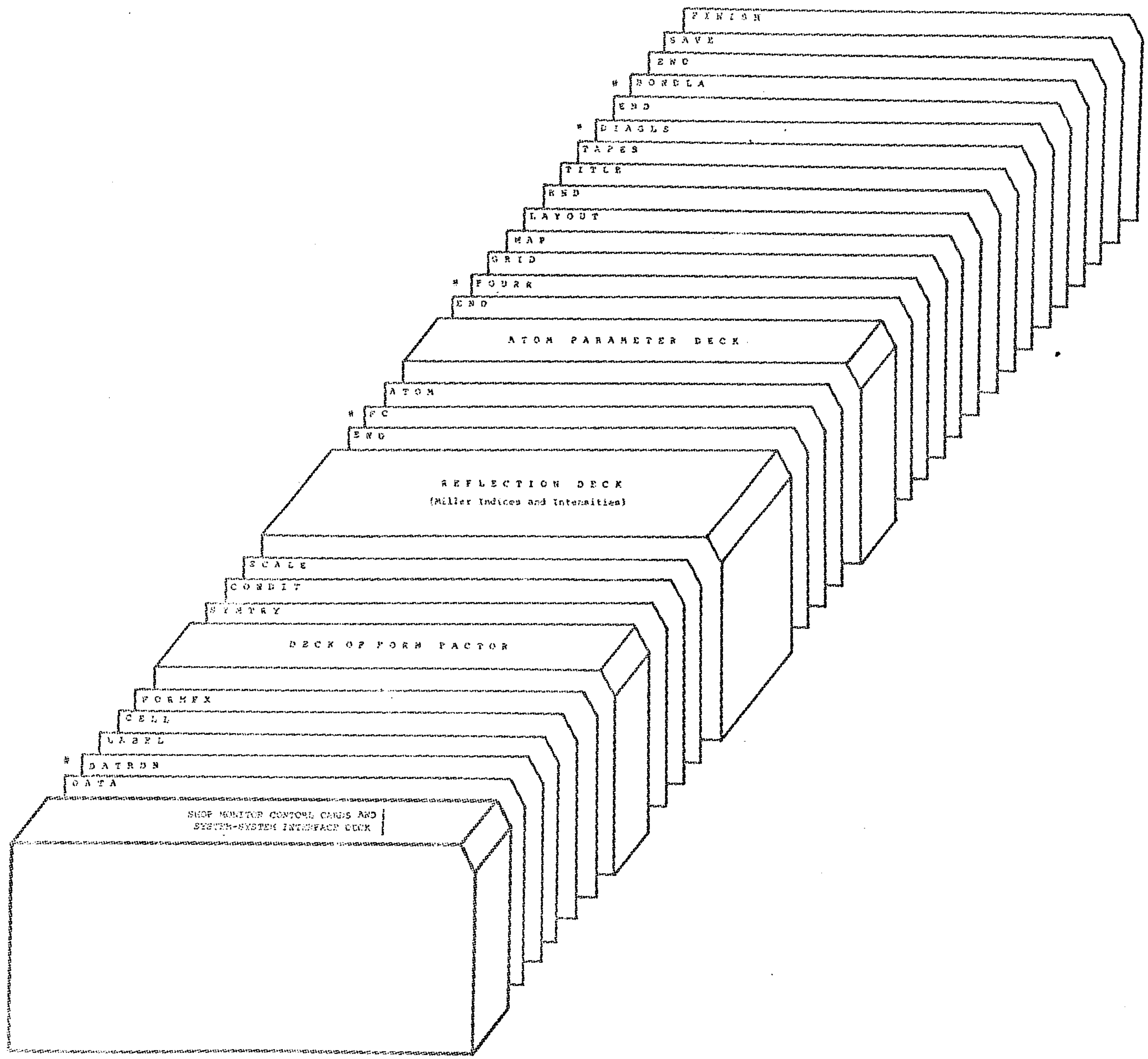
Division	Operational	In Planning and Checkout Stage
1. Systems Maintenance and Intersystem Compatibility	6	-
2. Data Gathering	4	-
3. Cell Parameter Determination	2	-
4. Preliminary Data Treatment	4	4
5. Structure Solving Programs	6	7
6. Parameter Refining Programs	4	3
7. Structure Interpretation and Presentation	7	5
8. Service Programs	3	6
9. Systems-Function Control	13	-
	49	25

Figure 4

Figure 5

EXAMPLE OF DATA DECK

FOR X-RAY-65 SYSTEM

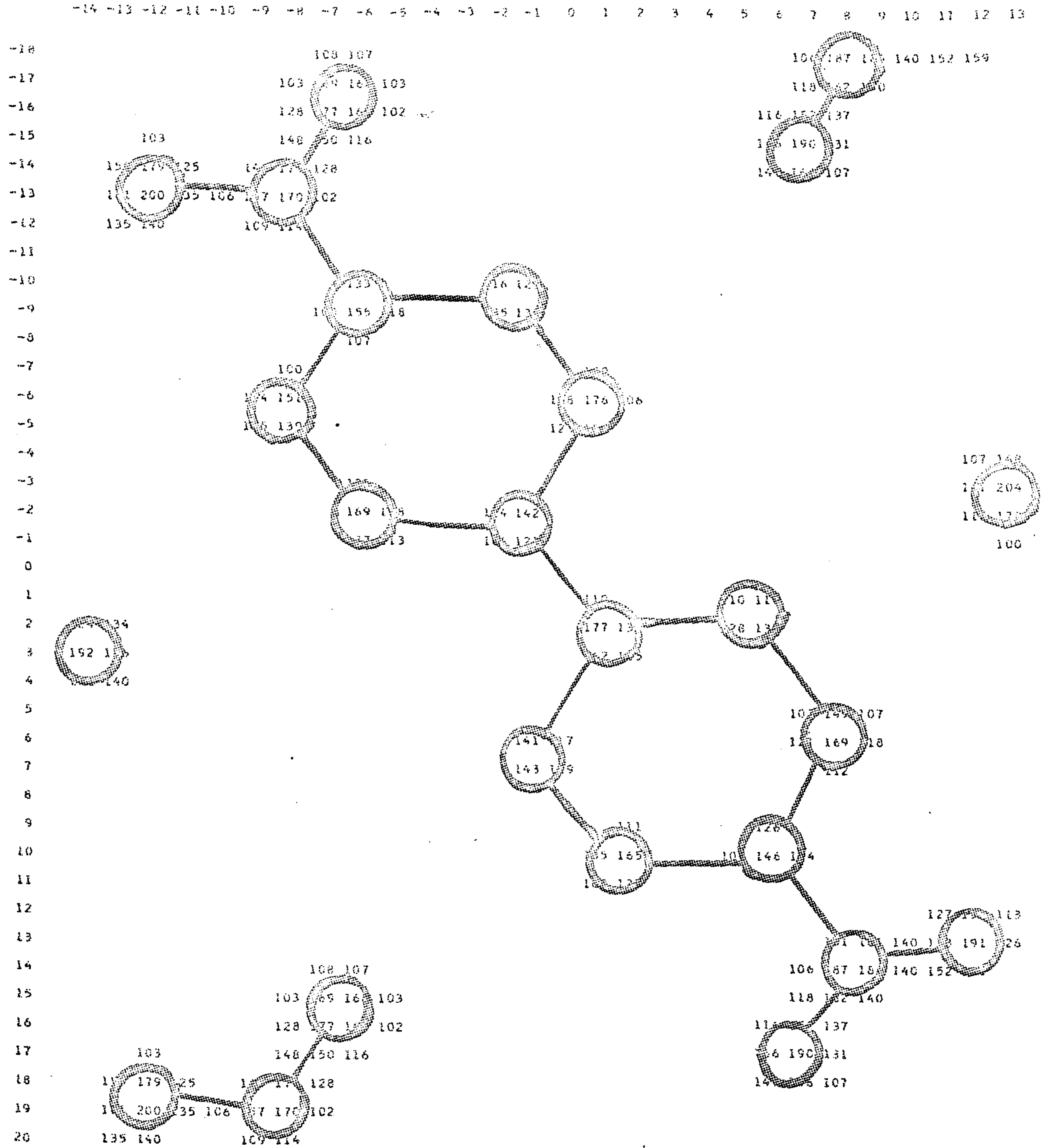


* PROGRAM CALLING CARDS

44   FO FOURIER   4,4(PRIME)-DINITRODIPHENYL AS TEST CASE. 23 DECEMBER 1964

Figure 6

Y IN 32NDS   Z IN 51STS   X = 0 12THS



The Numerical Solution of Non-Linear Functional Equations

Special Equations of Interest

Non-linear Integral Equations $\int_a^b K(s,t,x(t))\,dt = y(s)$

Non-linear Ordinary Differential Equations
(with suitable initial- or boundary conditions)

Non-linear Systems of n Equations in n Unknowns

General Setting

X, Y Banach spaces,

$F: X \to Y$ non-linear mapping from X into Y

Design and experiment with algorithms for solving $F(x) = 0$

Figure 7

Applications

Two-point boundary value problems, e.g., trajectory problems

Control problems

Flow problems

Minimization problems

Figure 8

Methods Currently Under Study

Local Methods

- Generalized Newton Method
- Generalized Secant Method
- Methods of Gauss - Seidel - and Jacobi - type for Non-linear Systems
- General Implicit Iterations

Global Algorithms

- Use of Perturbation Techniques
- Davidenko's Method
- Use of Imbedding Techniques

Figure 9

Particular Problems under Consideration

Newton's Method

- Conditions for monotonic convergence and their importance
- Influence of different approaches to the discretization problem
- Relations to Gradient-type methods

Gauss-Seidel and Jacobi type iterations

- Theoretical and Experimental comparison of asymptotic rates of convergence
- Global convergence

Secant Methods

- Theoretical and experimental convergence
- Sufficient conditions for convergence

Figure 10

Image Processing Research

Discrimination of Connected Regions

Discrimination of "Solid" from "Broken" Regions

Measures of Shape "Skeleton", "Capacity", "Frame"

Computer-Generated Patterns for Vision Research

Applications

Cloud Pattern Analysis

Contour Map Processing

Figure 11

Figure 12

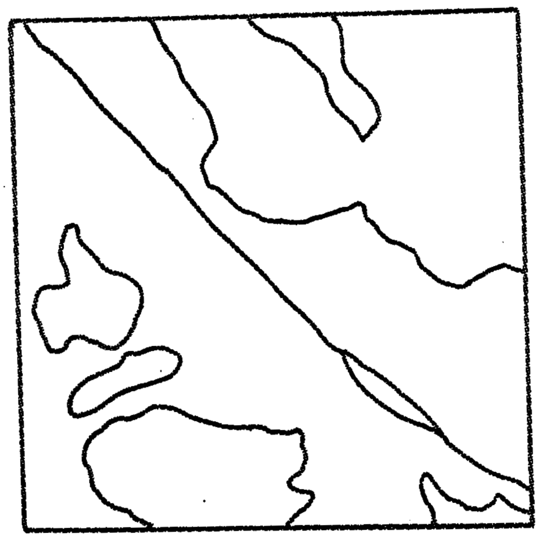


Figure 13

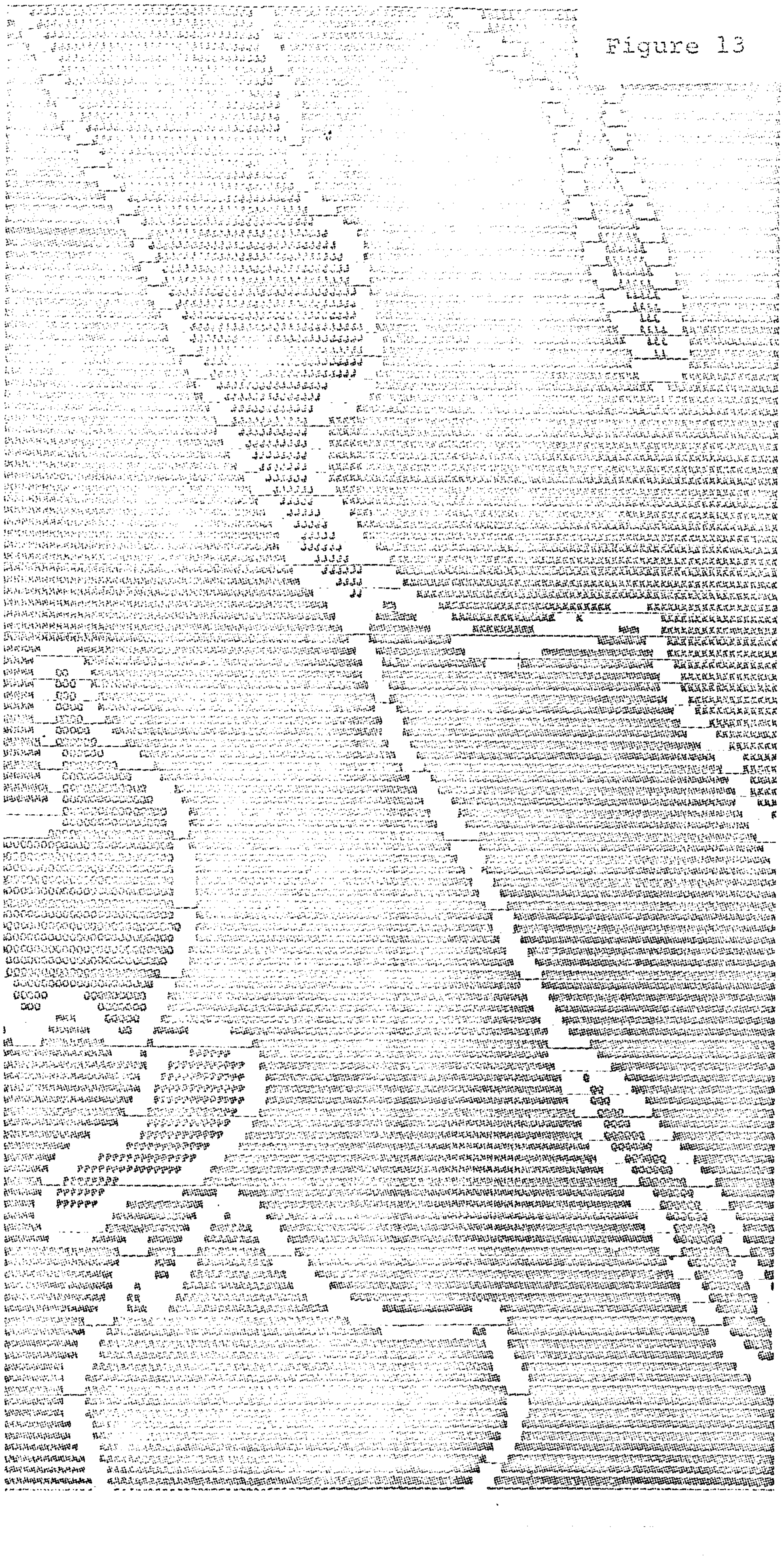
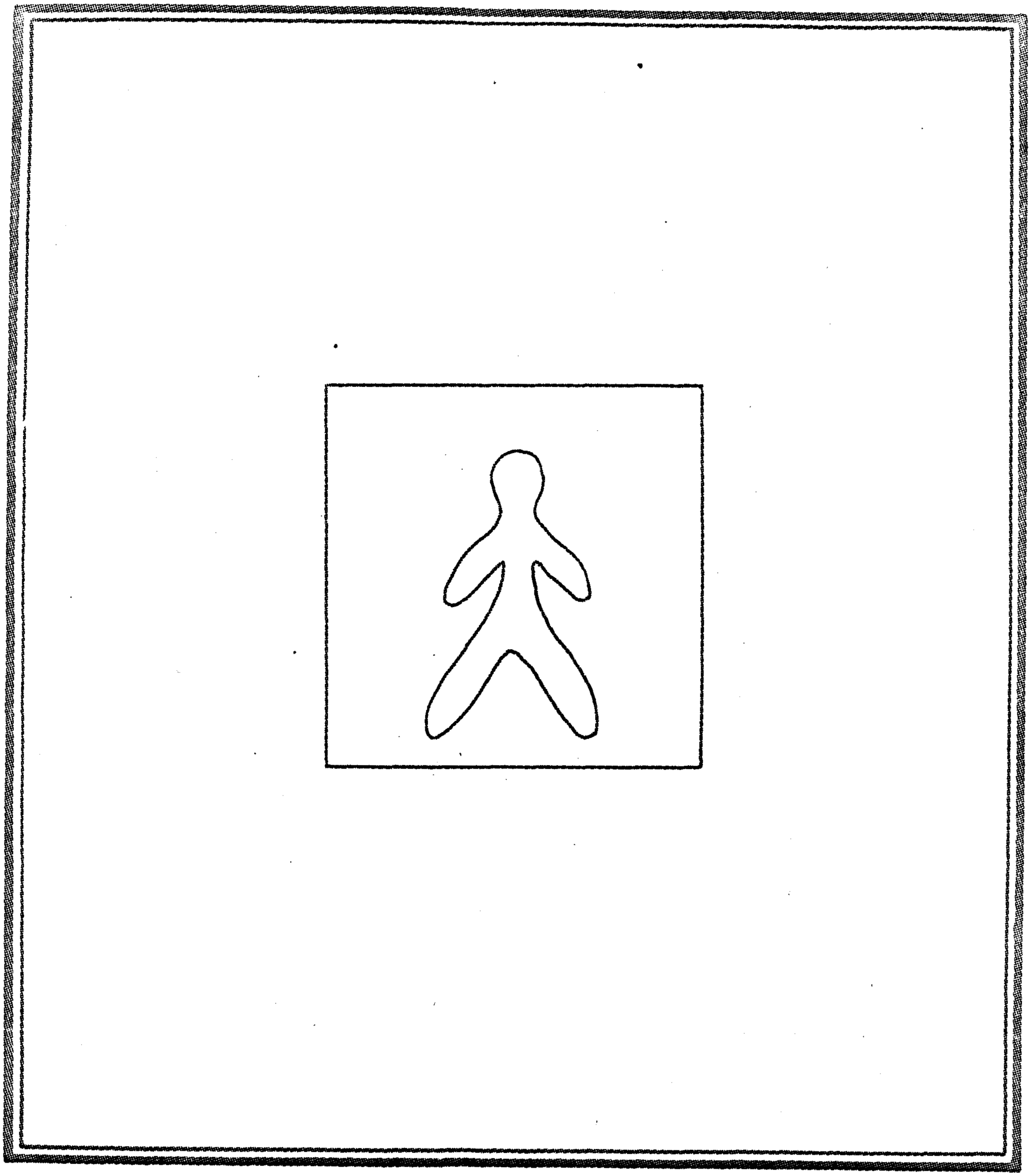


Figure 14



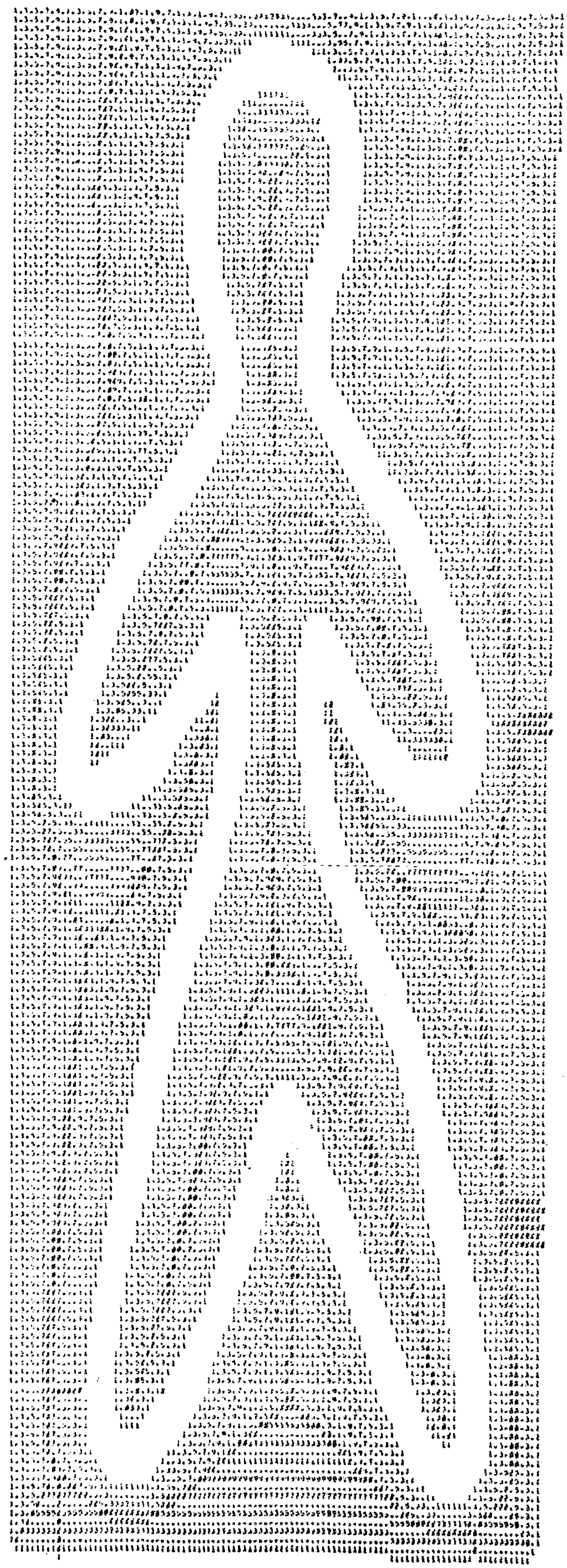
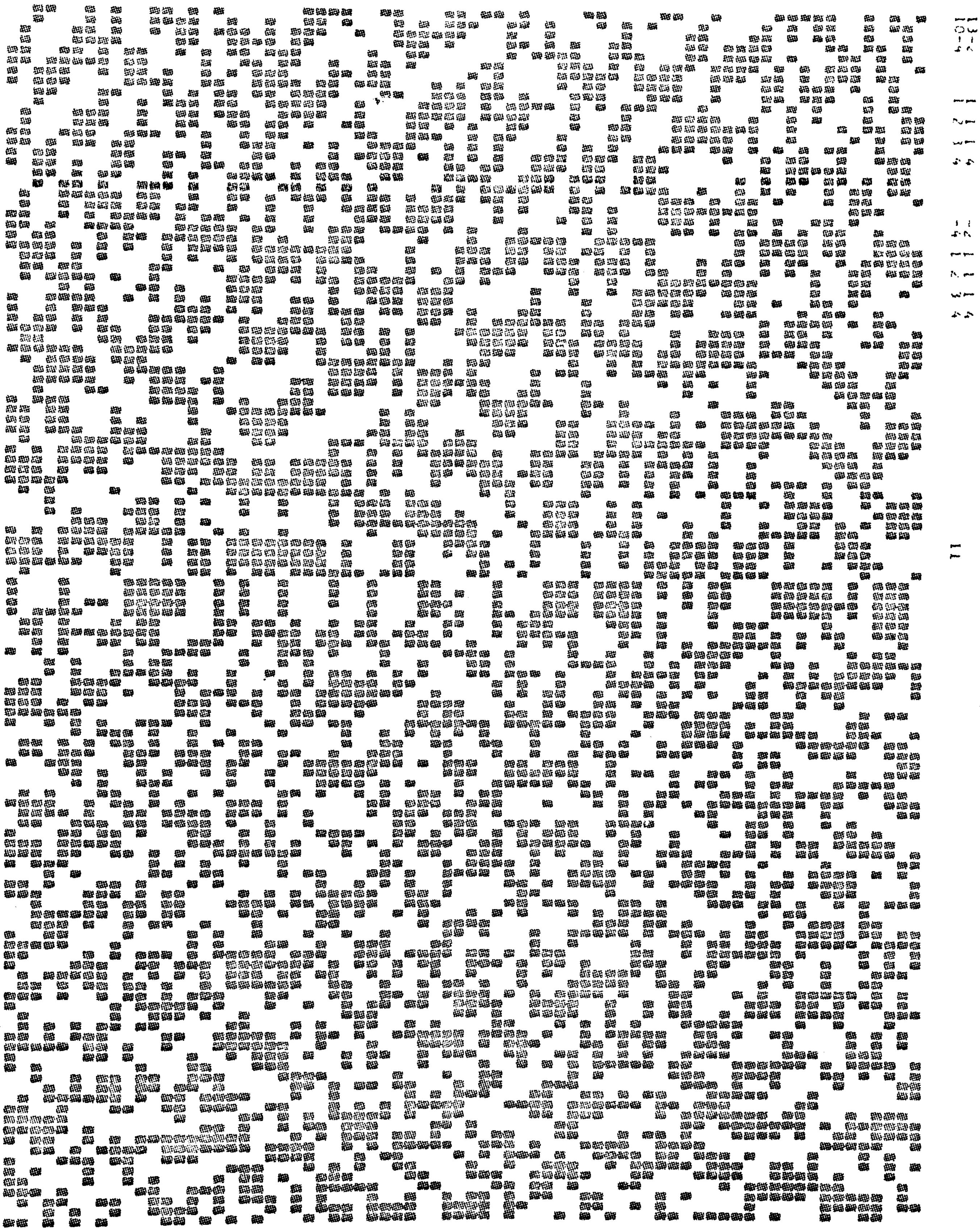


Figure 15

Figure 16



Computer-Oriented Research in Space Related Fields

Field	Department Represented	No. of Projects
1. Molecular Physics	Chemistry, Inst. for Molecular Physics	7
2. Nuclear Physics and Nuclear Engineering	Physics, Chemical Engineering	16
3. Particle and Field Physics	Physics	7
4. Physics and Engineering of Fluids	Inst. for Molecular Physics, Inst. for Fluid Dynamics, Physics, Chemical Engineering, Aeronautical Engineering	18
5. Mechanical and Elec. Engineering	Mechanical Engineering, Electrical Engineering	7
6. Other Disciplines	Astronomy, Physics, Mathematics, Psychology, Electrical Engineering	8

Figure 17

Figure 18

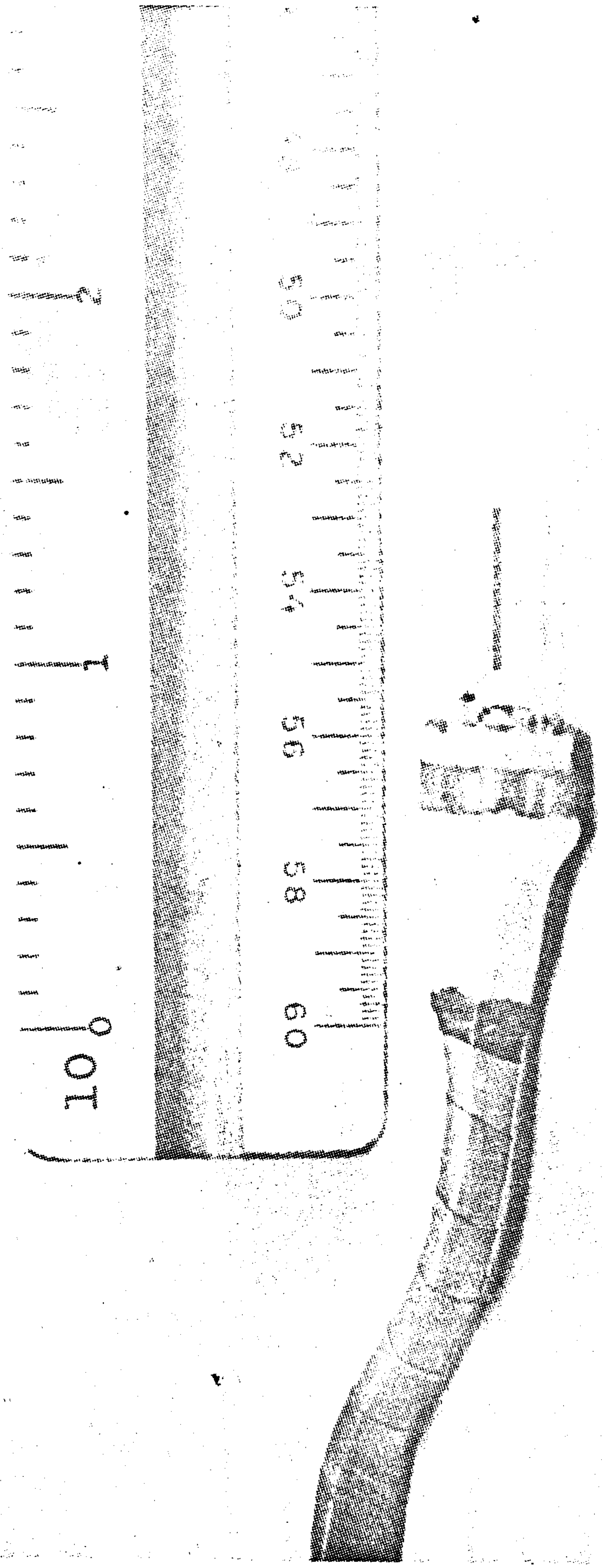
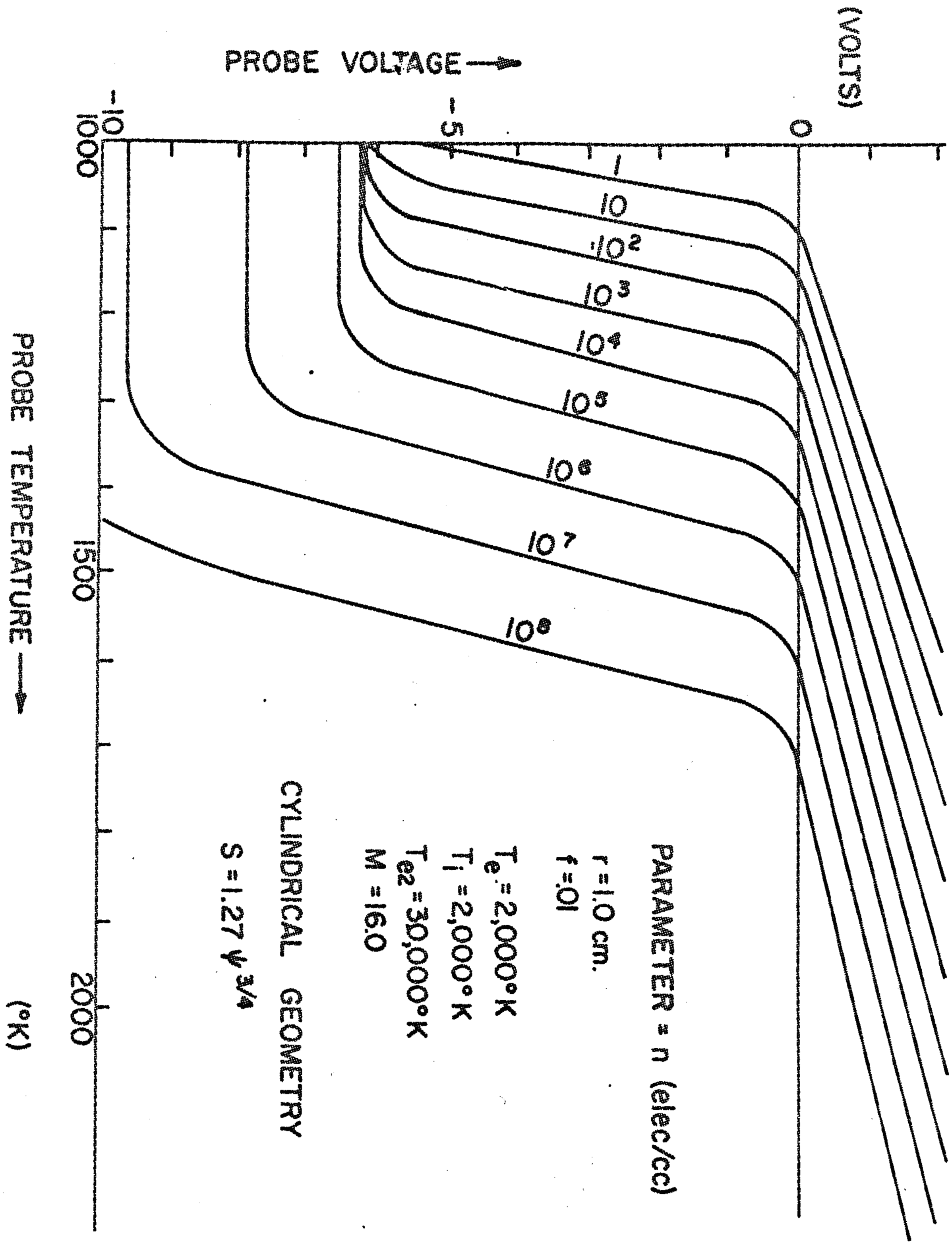
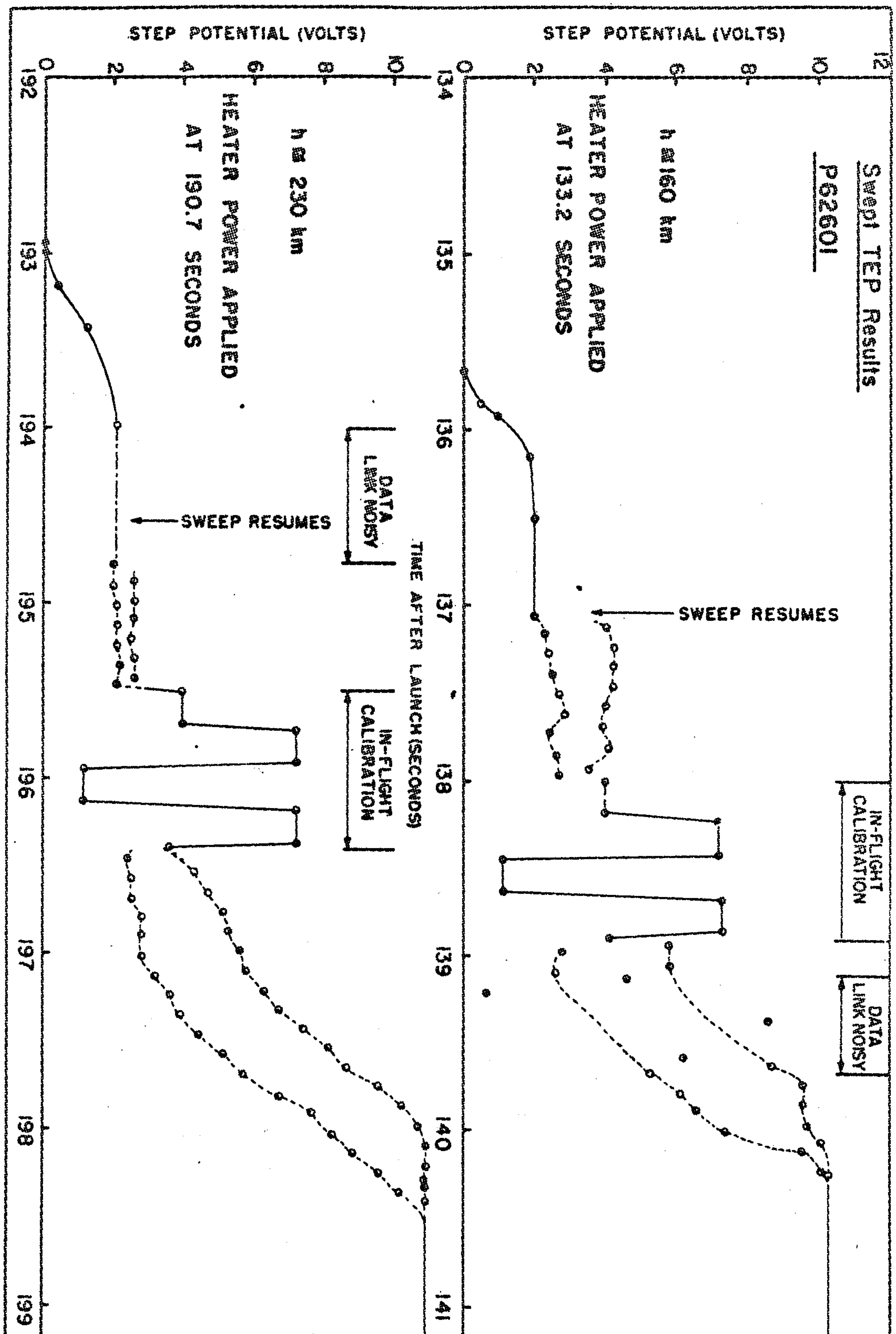


Figure 19

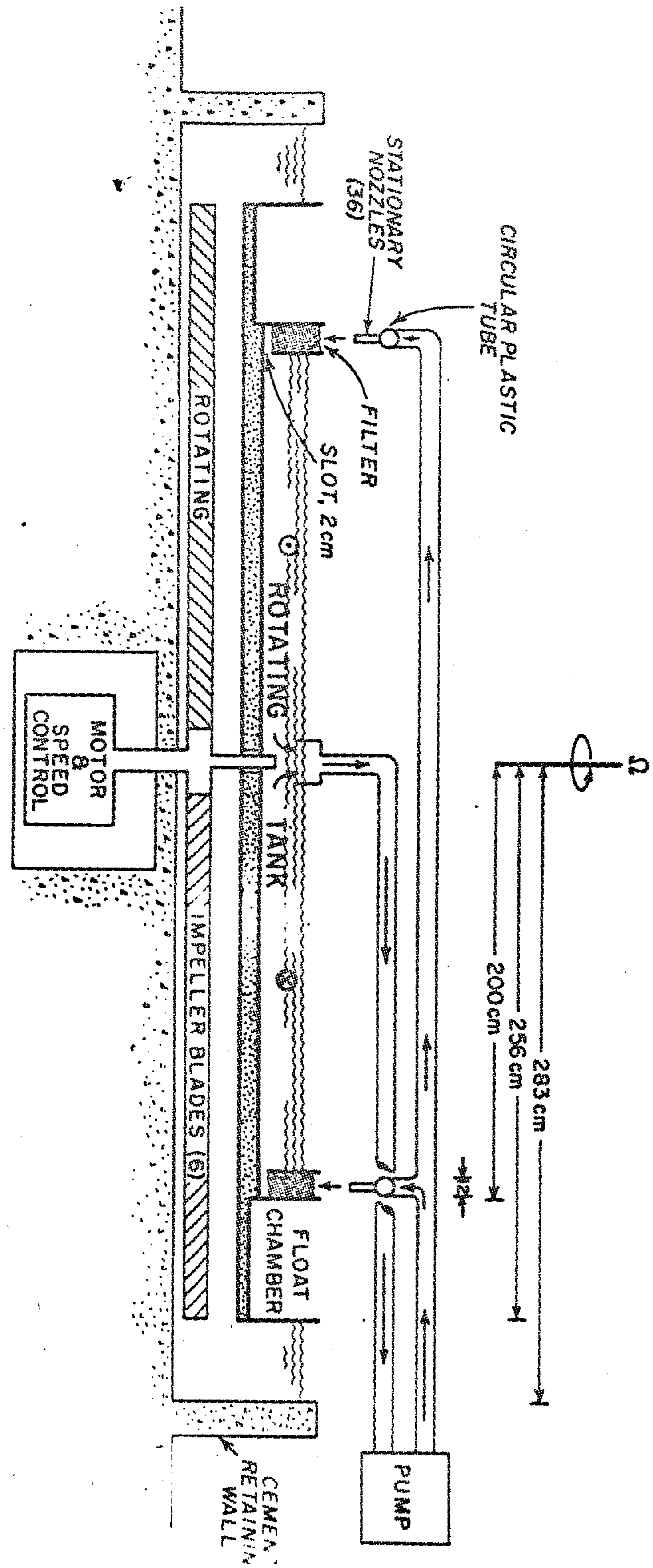


PROBE VOLTAGE
(VOLTS)
-10
-5
0
PROBE TEMPERATURE
(°K)
1000
1500
2000
1
10
10^2
10^3
10^4
10^5
10^6
10^7
10^8
PARAMETER = n (elec/cc)
r = 1.0 cm.
f = .01
T_e = 2,000°K
T_i = 2,000°K
T_{e2} = 30,000°K
M = 16.0
CYLINDRICAL GEOMETRY
S = $1.27\,\psi^{3/4}$

Figure 20



Swept TEP Results
P62601
h ≅ 160 km
HEATER POWER APPLIED
AT 133.2 SECONDS
SWEEP RESUMES
IN-FLIGHT CALIBRATION
DATA LINK NOISY
STEP POTENTIAL (VOLTS)
TIME AFTER LAUNCH (SECONDS)
h ≅ 230 km
HEATER POWER APPLIED
AT 190.7 SECONDS
SWEEP RESUMES
DATA LINK NOISY
IN-FLIGHT CALIBRATION
STEP POTENTIAL (VOLTS)



SCHEMATIC DIAGRAM OF THE 4-METER ROTATING TANK

Figure 22

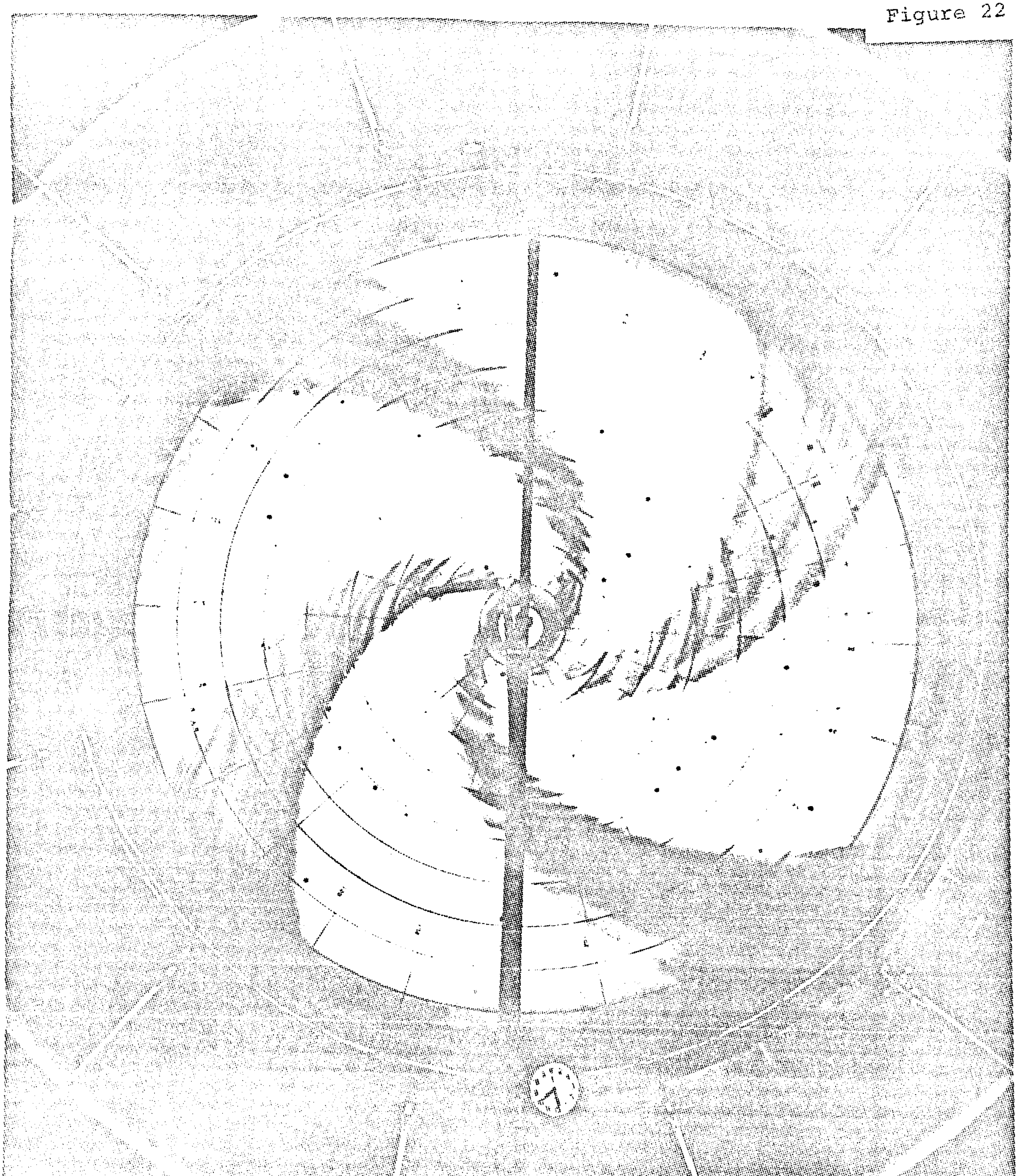
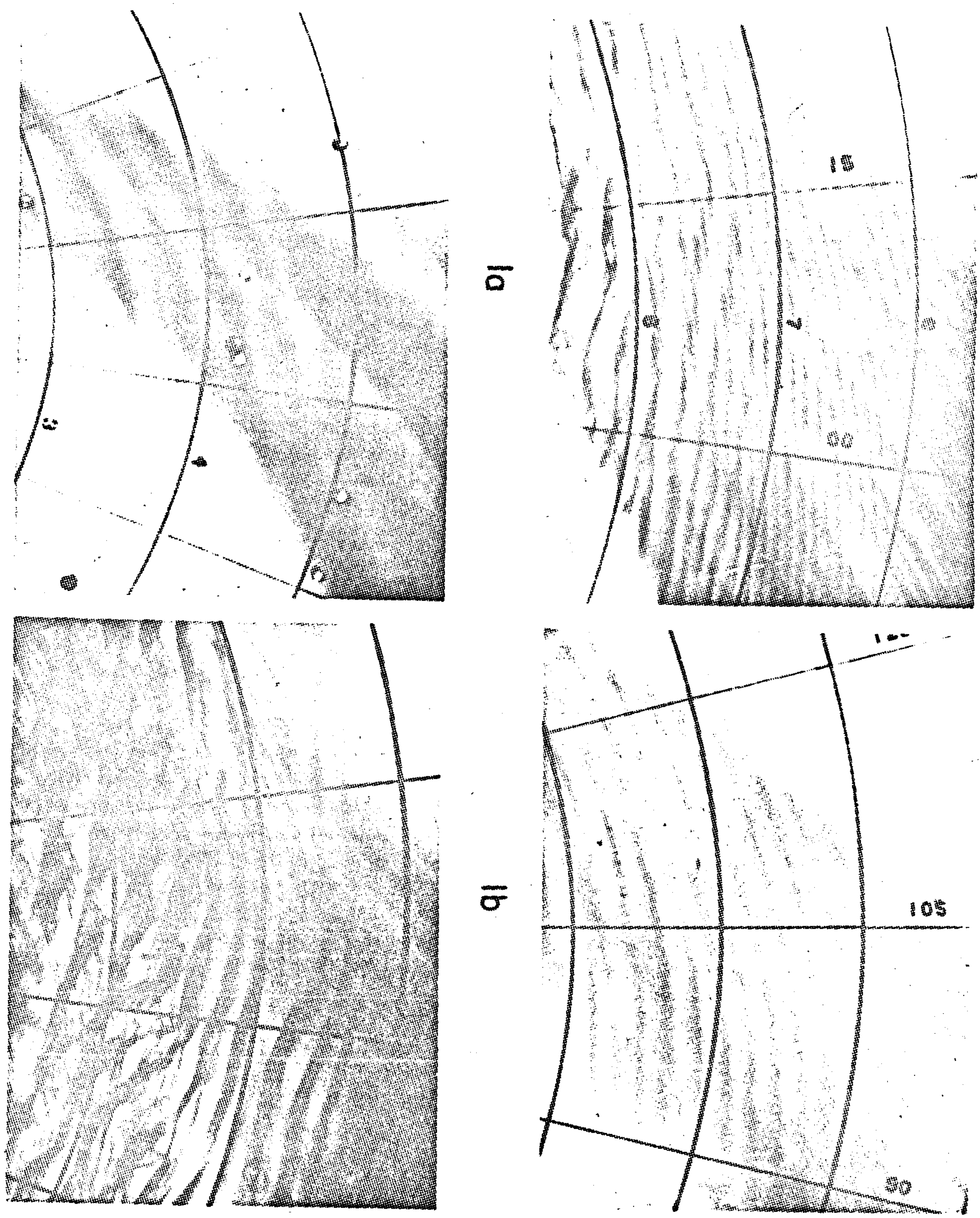
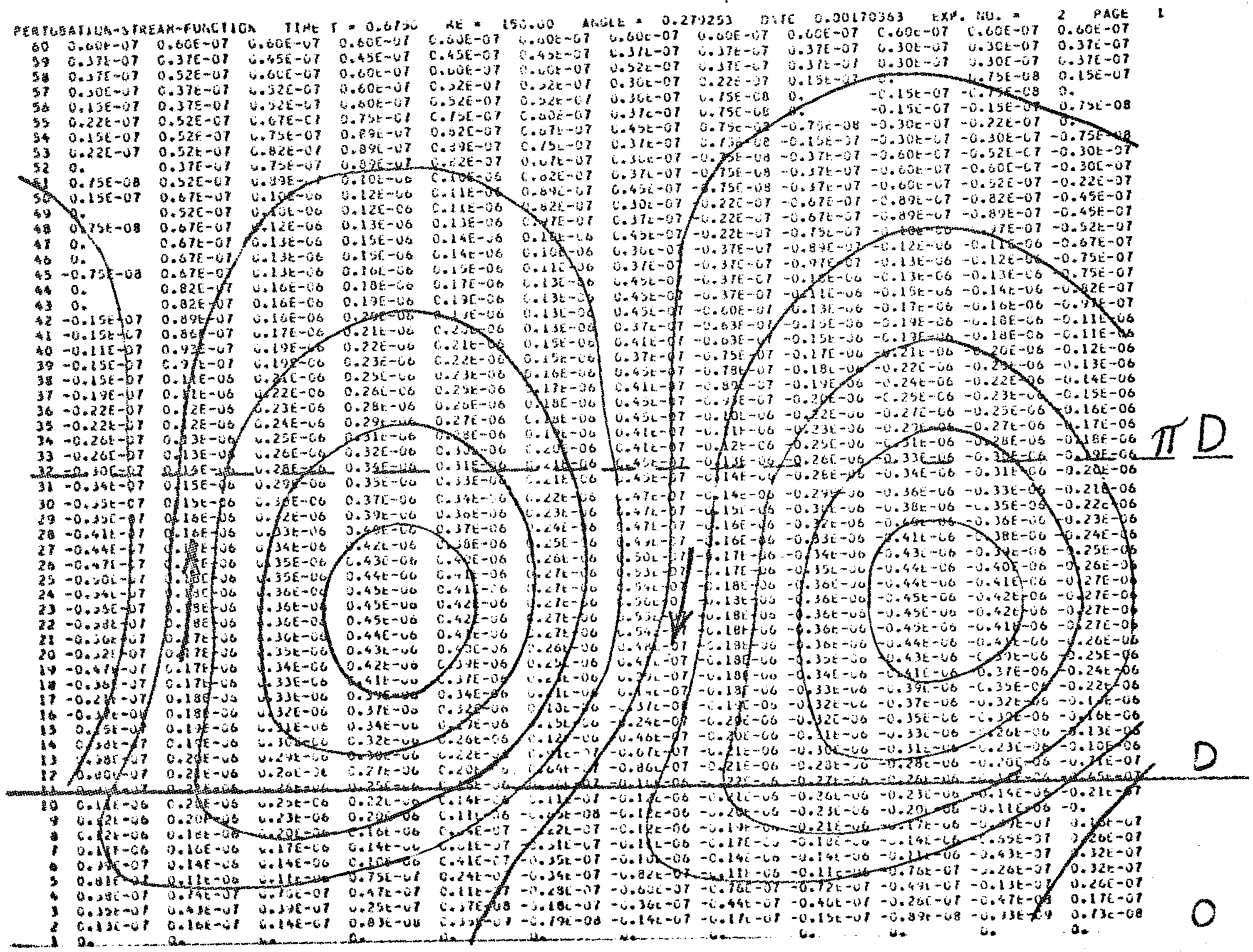


Figure 23





PERTURBATION STREAM FUNCTION

$Re = 150$, $Amp. = .45 \times 10^{-6}$

FIGURE 7